

Pseudospin bases for a model of $\text{Cu:Bi}_2\text{Se}_3$

Sungkit Yip

Institute of Physics and Institute of Atomic and Molecular Sciences
Academia Sinica

128 Academia Road, Sec 2, Nankang, Taipei 115, Taiwan.

E-mail: yip@phys.sinica.edu.tw

Abstract.

We consider the construction of pseudospin bases for a time-reversal and inversion symmetric system, illustrated by a model for $\text{Cu:Bi}_2\text{Se}_3$. Different methods and bases are compared.

PACS numbers: 74.20.-z, 74.20.Rp, 73.20.At

1. Introduction

Bi_2Se_3 , a well-established topological insulator, becomes superconducting when doped or intercalated with copper [1, 2, 3] or other elements such as strontium [4]. There is much debate on the superconducting state for this material. Initially the favorite was the fully gapped odd-parity state with A_{1u} symmetry respecting all rotational symmetries of the crystal [3, 5, 6]. However, possibilities later considered include also conventional s-wave [7, 8], and more recently, broken rotational symmetry odd parity states [9, 10, 11, 12, 13]. Moreover, the superconducting properties of this material have some unusual characteristics [14, 15]. The mechanism for superconductivity is also hotly debated [5, 16, 17].

Early on, theoretical works on superconductivity in this material [5, 18, 19, 20] started with effective multi-orbital model motivated by the topological insulator Bi_2Se_3 itself. Thus the minimum model of the normal state part of the Hamiltonian H_N contains four degrees of freedom, resulting from two orbitals of different parity together with two spins degree of freedom. For example, we can write, following [5]

$$H_N(\vec{k}) = m\sigma_x + v_z k_z \sigma_y + v\sigma_z(k_x s_y - k_y s_x) \quad (1)$$

where $\sigma_z = \pm 1$ represents the two (mainly) p_z orbitals in the quintuple layer of Bi_2Se_3 , and \vec{s} the spin. Here \vec{k} , k_x , k_y , k_z represent the wavevector and its components, v_z , v are velocities. m is a quantity of dimension energy distinguishing the topologically trivial (commonly taken as $m > 0$) and the non-trivial cases ($m < 0$). For simplicity, we shall confine ourselves to the vicinity of $\vec{k} = 0$. (This model is thus valid only for very small doping. The main point we would like to discuss in this paper is the methodology of finding the pseudospin basis. Complications such as higher order terms in \vec{k} , as well as the fact that the Fermi surface seemingly changes shape substantially for larger doping [21], would not be considered here. As noted before (e.g. [22]), the model (1) thus has symmetry $D_{\infty,h}$ which is actually higher than D_{3d} of the crystal.) An important feature of this model is that spins and orbital degrees of freedom are coupled, as this is necessary to describe the topological insulator. Expressing superconducting pairing also in terms of these orbitals and spins, properties of the superconductor can be directly evaluated (e.g. [5, 18, 19, 20]). While this approach is perfectly alright by itself, the connection with the previous superconductivity literature [23, 24, 25, 26, 27, 28, 29, 30], in particular those on heavy fermion superconductivity where spin-orbit coupling also cannot be ignored, is unclear. There the approach was to express electronic states near the Fermi surface in the normal state in terms of pseudospins, (note that these then depend only on the normal state Hamiltonian), and Cooper-pairing between pseudospin states at opposite momenta then considered. One can connect these two pictures by, starting from say the multi-orbital model, explicitly construct this pseudospin basis set for the electrons near the Fermi surface, and then express the pairing in terms of that between the pseudospins at $\pm\vec{k}$. For the basis set to be “more useful” in the sense that connection with the earlier literature [23, 24, 25, 26, 27, 28, 29, 30] can be made, these

pseudospin states must satisfy certain symmetry criteria, in particular those imposed by time-reversal, parity and rotational symmetries.

At a typical point (labeled by the momentum \vec{k}) on the Fermi surface, there are two degenerate states since the crystal obeys time-reversal and parity symmetries. Given the Hamiltonian, it is straight-forward to find two orthonormal states, say $|\vec{k}, \alpha'\rangle$ and $|\vec{k}, \beta'\rangle$, at each point on the Fermi surface. Symmetry operations map states from one point of the Fermi surface to a linear combination of those at another (and for some operations, the same) point. The task at hand is to find a suitable unitary transformation among these two states $|\vec{k}, \alpha'\rangle$ and $|\vec{k}, \beta'\rangle$ to form two new ones $|\vec{k}, \alpha\rangle$ and $|\vec{k}, \beta\rangle$ so that the latter would transform the same way as “up” and “down” spins under the symmetry operations. ‡ One such explicit construction for the model (1) was given by the author himself [22], and another, slightly later, by Fu and his coworkers [31, 32, 10]. The two pseudospin bases differ slightly, reflecting the non-uniqueness of their choice.

With these constructions, one can, for example, now re-express the pairings $\Delta_{1,2,3,4}$ introduced in [5], originally in terms of orbitals and spins of (1), in terms of the basis functions listed in, e.g. [26, 27, 28]. § Many properties of these superconducting states are then directly evident. Some examples are given in [22, 10] (see also [33]).

The purpose of the present paper is to discuss the relation between these two methods ([22] on one hand and [31, 32, 10] on the other) of constructing the pseudospins. In the beginning of the next section, we first review the essence of both methods. We then illustrate in section 2.1 that a slight modifications of [22] would amount to a method and hence results identical to [31, 32, 10]. We then construct in section 2.2 yet another basis based on the same principle in [22]. The advantages and disadvantages of the different pseudospin bases are discussed.

2. Review of the methods in [22] and [31, 32, 10]

We briefly review the methods in [22] and [31, 32, 10]. We shall do this in the context of the two-orbital two-spin model of (1), though the basic points that we are making are completely general. For (1), the eigenstates $|\vec{k}, \alpha'\rangle$ and $|\vec{k}, \beta'\rangle$ can be represented as column vectors of 4 entries. The transformation relations, under rotations say, among these states, can look unfamiliar and the construction of $|\vec{k}, \alpha\rangle$ and $|\vec{k}, \beta\rangle$ not immediately obvious. To overcome this point, the author [22] made use of the fact that the magnetic moment must transform like a pseudo-vector. Pretending that this magnetic moment

‡ Actually, to discuss superconductivity, it is sufficient that the Cooper pairs have the proper transformations: see, e.g., [26]. Hence our construction here has imposed more constraints than is necessary. However, we shall keep to this more stringent requirement for easier presentation.

§ Rigorously speaking, the symmetry of Bi_2Se_3 is D_{3d} , and Cooper-pair basis functions for this symmetry were not listed in the above references. However, since D_{3d} is a subgroup of D_{6h} , the pair basis functions can be read off from these references by identifying B_1 with A_1 , B_2 with A_2 , and E_2 with E_1 (separately for even and odd parities g and u). For example, in E_u , basis functions listed under E_{1u} and E_{2u} are both acceptable (though some care is needed to identify the correct partners, c.f., e.g., [30]).

simply arises from the spin, he was led to consider the spin operator \vec{s} within the two-dimensional space generated by $|\vec{k}, \alpha'\rangle$ and $|\vec{k}, \beta'\rangle$. Thus $s_{x,y,z}$ become 2×2 matrices, and are then linear combinations of $\rho'_{x,y,z}$, the Pauli matrices in $|\vec{k}, \alpha'\rangle$ and $|\vec{k}, \beta'\rangle$ space. In general $\rho'_{x,y,z}$ would fail to transform as the x, y, z components of a pseudo-vector. The required proper basis $|\vec{k}, \alpha\rangle$ and $|\vec{k}, \beta\rangle$, can be easily identified, since the Pauli matrices $\rho_{x,y,z}$ in this space is related to $\rho'_{x,y,z}$ by a rotation which is related to the unitary transformation between $|\vec{k}, \alpha\rangle$, $|\vec{k}, \beta\rangle$ and $|\vec{k}, \alpha'\rangle$, $|\vec{k}, \beta'\rangle$. As a byproduct, one also obtains an expression of the magnetic moment of quasiparticles in terms of the pseudospins. [22]

Actually, the general form for the magnetic moment corresponding to this two-orbital model is more complicated. As pointed out in [34], the magnetic moment, in the notations of (1), is a linear combination of \vec{s} and $\sigma_x \vec{s}$ (more precise statements below). One is actually free to choose any linear combination between these two quantities to carry out the procedure outlined above, since they are both pseudovectors. A slightly different pseudospin basis would be obtained, and this reflects the non-uniqueness of the choice of the pseudospin basis.

On the other hand, Fu and his coworkers [31, 32, 10] introduce what they called “manifestly covariant Bloch basis” (MCBB). They construct this by first identifying a point which they regard as invariant under the relevant symmetries. By demanding that $|\vec{k}, \alpha\rangle$ and $|\vec{k}, \beta\rangle$ at this point be proportional to a real number times a wavefunction consisting of spin up and down respectively, they show that this basis automatically possesses the required transformation, in particular rotational properties. For the example of (1), they regard the system as invariant under the parity operation σ_x . In this way, a pseudospin basis was constructed [31, 32, 10].

A moment of thought shows that, in the method used by the author [22], if the operator $(1 + \sigma_x)\vec{s}$ was employed instead of \vec{s} in [22], the basis constructed would then just be MCBB. (Lest this is not obvious, an explicit demonstration would be given in Sec 2.1.). Viewed entirely mathematically, in both [22] and [31, 32, 10], the procedures used amount to reducing the effective wavefunctions to be only column matrices of two entries. In [22], it was done by choosing a pseudovector operator and evaluating it in the Hilbert space $|\vec{k}, \alpha'\rangle$ and $|\vec{k}, \beta'\rangle$, and one worked with 2×2 matrices rather than wavefunctions. In [31, 32, 10], it was done by identifying a particular symmetry operation that does so. The choice needed for the procedure in [22] can always be chosen as \vec{s} or any suitable modifications. The same choice can be used for more general situations, such as when the model contains more orbitals than two, or when the symmetry operations contain screw axes or glide planes. For [31, 32, 10], the parity operator may not directly be able to reduce the wavefunctions to a two-component one, though one is likely able to identify a suitable generalization.

2.1. MCBB via the method of [22]

Now we turn to explicit calculations to verify our claim in the last paragraph, that is, the pseudospins constructed using the method of [22] with a slightly different operator would yield directly the MCBB pseudospins of [31, 32, 10]. As mentioned, for (1), generally the magnetic moment \vec{m} is a linear combination \vec{s} and $\vec{\sigma}_x \vec{s}$. More precisely, its components can be written as,

$$m_z = g_{1z} \frac{1 + \sigma_x}{2} s_z + g_{2z} \frac{1 - \sigma_x}{2} s_z \quad (2)$$

$$m_{x,y} = g_{1p} \frac{1 + \sigma_x}{2} s_{x,y} + g_{2p} \frac{1 - \sigma_x}{2} s_{x,y} \quad (3)$$

These equations are simply eq (45) of [34] adopted to the notations here of (1). (Our $g_{1z} \dots g_{2p}$ are thus the same as those in [34]). For convenience, we have dropped factors of $\frac{\mu_B}{2}$ where μ_B is the Bohr magneton to simplify (2), (3) and other equations for \vec{m} below. We shall write $m_z = m_{1z} + m_{2z}$ where m_{1z} and m_{2z} are the two contributions proportional to g_{1z} and g_{2z} in (2) and similarly for m_x and m_y for (3).

We now construct the pseudospin basis for the model (1) using the same procedure as in [22] with only the difference that \vec{m}_1 would be used rather than \vec{s} there. Let us first recall that it is sufficient to construct the pseudospins for half of the Fermi sphere (which we shall refer to as “northern hemisphere”), since we always require [22], for any given \vec{k} ,

$$|-\vec{k}, \alpha\rangle = P|\vec{k}, \alpha\rangle \quad (4)$$

and

$$|\vec{k}, \beta\rangle = TP|\vec{k}, \alpha\rangle \quad (5)$$

(hence also $|-\vec{k}, \beta\rangle = P|\vec{k}, \beta\rangle$) where P, T are the parity and time-reversal operators respectively. We shall adopt the sign convention $T|s_z = 1\rangle = |s_z = -1\rangle$ (thus $T|s_z = -1\rangle = -|s_z = 1\rangle$) for the spin wavefunctions. For the evaluations below, it is useful to note that $P_+ \equiv \frac{1+\sigma_x}{2}$ is a projection operator: $P_+^2 = P_+$, and we have $m_{1z} = g_{1z} P_+ s_z$ and similarly for the x and y components. For a given point \vec{k} on the Fermi surface, let us start with the two degenerate solutions [22] at \vec{k} :

$$|\vec{k}, \alpha'\rangle \equiv \frac{1}{\sqrt{2}\mathcal{N}_{\vec{k}}} e^{i\vec{k}\cdot\vec{r}} \begin{pmatrix} E_{\vec{k}} + vk_{\parallel} \\ m + iv_z k_z \end{pmatrix} \begin{pmatrix} 1 \\ ie^{i\phi_{\vec{k}}} \end{pmatrix} \quad (6)$$

$$|\vec{k}, \beta'\rangle \equiv \frac{1}{\sqrt{2}\mathcal{N}_{\vec{k}}} e^{i\vec{k}\cdot\vec{r}} \begin{pmatrix} m - iv_z k_z \\ E_{\vec{k}} + vk_{\parallel} \end{pmatrix} \begin{pmatrix} ie^{-i\phi_{\vec{k}}} \\ 1 \end{pmatrix} \quad (7)$$

We are using the notation that the first column matrix denotes the part in orbital space and the second part denotes the spin space. Here $E_{\vec{k}}$ is the energy of the particle (which is $(m^2 + v_z^2 k_z^2 + v^2 k_{\parallel}^2)^{1/2}$ for positive energies), and $\mathcal{N}_{\vec{k}} \equiv [2E_{\vec{k}}(E_{\vec{k}} + vk_{\parallel})]^{1/2}$ is a renormalization factor. Here k_{\parallel} , $\phi_{\vec{k}}$ are respectively the magnitude and azimuthal angle of the momentum in the x-y plane. Note that we have already chosen $|\vec{k}, \beta'\rangle = TP|\vec{k}, \alpha'\rangle$.

Following the procedure in [22], we shall evaluate \vec{m}_1 and hence $P_1\vec{s}$ in the $|\vec{k}, \alpha'\rangle$ $|\vec{k}, \beta'\rangle$ space. It is convenient to first evaluate $P_+|\vec{k}, \alpha'\rangle$ and $P_+|\vec{k}, \beta'\rangle$, since for example $\langle\vec{k}, \alpha'|P_+\vec{s}|\vec{k}, \alpha'\rangle = \langle\vec{k}, \alpha'|P_+\vec{s}P_+|\vec{k}, \alpha'\rangle$. We easily find (suppressing the plane wavefactors $e^{i\vec{k}\cdot\vec{r}}$ from now on)

$$P_+|\vec{k}, \alpha'\rangle = \frac{W_{\vec{k}}}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ ie^{i\phi_{\vec{k}}} \end{pmatrix} \quad (8)$$

and

$$P_+|\vec{k}, \beta'\rangle = \frac{W_{\vec{k}}}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} ie^{-i\phi_{\vec{k}}} \\ 1 \end{pmatrix} \quad (9)$$

Here

$$W_{\vec{k}} \equiv \frac{(E_{\vec{k}} + vk_{\parallel}) + (m + iv_z k_z)}{\sqrt{2}\mathcal{N}_{\vec{k}}} \quad (10)$$

is a coefficient resulting from the projection P_+ . We easily get

$$|W_{\vec{k}}| = \left[\frac{1}{2}\left(1 + \frac{m}{E_{\vec{k}}}\right)\right]^{1/2}. \quad (11)$$

If we consider the branch of (1) with $E_{\vec{k}} > 0$, then for $m > 0$, $|W_{\vec{k}=0}| = 1$, which reflects that this state corresponds to even parity in the model of (1). If $m < 0$, then $|W_{\vec{k}=0}| = 0$. At the chemical potential μ , $|W_{\vec{k}}| = [\frac{1}{2}(1 + \frac{m}{\mu})]^{1/2}$. (For more general models than eq (1), $|W_{\vec{k}}|$ can still depend on the direction of \vec{k} even on the Fermi surface.) For Bi_2Se_3 which has band inversion $m < 0$, $|W| < 1/\sqrt{2}$ at the Fermi level if it is electron-doped ($\mu > 0$). To simplify our notations here and below, we shall leave out the subscript \vec{k} for $W_{\vec{k}}$ whenever no confusion can arise.

Note that

$$|\hat{k}+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ ie^{i\phi_{\vec{k}}} \end{pmatrix} \quad (12)$$

$$|\hat{k}-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} ie^{-i\phi_{\vec{k}}} \\ 1 \end{pmatrix} \quad (13)$$

are respectively the spin wavefunctions for spins along $\pm\hat{z} \times \hat{k}$. Since $\langle\hat{k} \pm |s_z|\hat{k} \pm\rangle = 0$ whereas $\langle\hat{k} \mp |s_z|\hat{k} \pm\rangle = \mp ie^{\pm i\phi_{\vec{k}}}$, we easily find that m_{1z} has the following matrix form in $|\vec{k}, \alpha'\rangle$ $|\vec{k}, \beta'\rangle$ space:

$$\begin{aligned} m_{1z}(\vec{k}) &\rightarrow g_{1z} \begin{pmatrix} \langle\vec{k}, \alpha'|P_1 s_{1z}|\vec{k}, \alpha'\rangle & \langle\vec{k}, \alpha'|P_1 s_{1z}|\vec{k}, \beta'\rangle \\ \langle\vec{k}, \beta'|P_1 s_{1z}|\vec{k}, \alpha'\rangle & \langle\vec{k}, \beta'|P_1 s_{1z}|\vec{k}, \beta'\rangle \end{pmatrix} \\ &= g_{1z} \begin{pmatrix} 0 & ie^{-i\phi_{\vec{k}}} W^{*2} \\ -ie^{i\phi_{\vec{k}}} W^2 & 0 \end{pmatrix} \end{aligned} \quad (14)$$

The eigenvalues of this matrix are $\pm|W|^2$. We would like to find a new basis $|\vec{k}, \alpha\rangle$ and $|\vec{k}, \beta\rangle$ such that the right hand side of (14) has the same transformation of the z component of a Pauli matrix. Evidently, we can just “diagonalize” (14) (so that

$m_{1z} \propto \rho_z$) if we take $|\vec{k}, \alpha\rangle \propto |\vec{k}, \alpha'\rangle - ie^{i\phi_{\vec{k}}} \frac{W^2}{|W|^2} |\vec{k}, \beta'\rangle$. Keeping $|\vec{k}, \beta\rangle = TP|\vec{k}, \alpha\rangle$, we have then

$$m_{1z}(\vec{k}) = g_{1z}|W|^2\rho_z \quad (15)$$

where we are using $\rho_{x,y,z}$ to denote Pauli matrices in $|\vec{k}, \alpha\rangle$ and $|\vec{k}, \beta\rangle$ space. Now ρ_z has the correct transformation property. The overall phase factor for $|\vec{k}, \alpha\rangle$ must further be chosen so that $\rho_{x,y}$ also transform correctly. The necessary choice can be seen to be

$$|\vec{k}, \alpha\rangle = \frac{1}{\sqrt{2}} \left(\frac{W^*}{|W|} |\vec{k}, \alpha'\rangle - ie^{i\phi_{\vec{k}}} \frac{W}{|W|} |\vec{k}, \beta'\rangle \right) \quad (16)$$

and hence (via (5))

$$|\vec{k}, \beta\rangle = \frac{1}{\sqrt{2}} \left(-ie^{-i\phi_{\vec{k}}} \frac{W^*}{|W|} |\vec{k}, \alpha'\rangle + \frac{W}{|W|} |\vec{k}, \beta'\rangle \right) \quad (17)$$

With this choice, we have then

$$m_{1x}(\vec{k}) = g_{1p}|W|^2\rho_x \quad (18)$$

$$m_{1y}(\vec{k}) = g_{1p}|W|^2\rho_y \quad (19)$$

ensuring correct transformation properties of $\rho_{x,y,z}$. From (16), we can verify explicitly

$$P_+|\vec{k}, \alpha\rangle = \frac{|W|}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (20)$$

hence involves only spin up $|s_z = 1\rangle$. This basis thus satisfy the criteria of MCBB of [31]. One can indeed verify explicitly from (16) that we have (in the basis $|\sigma_z, s_z\rangle = |1, 1\rangle, |1, -1\rangle, |-1, 1\rangle, |-1, -1\rangle$)

$$|\vec{k}, \alpha\rangle = \frac{1}{2E_{\vec{k}}[1 + \frac{m}{E_{\vec{k}}}]^{1/2}} \begin{pmatrix} E_{\vec{k}} + m - iv_z k_z \\ ivk_{\parallel} e^{i\phi_{\vec{k}}} \\ E_{\vec{k}} + m + iv_z k_z \\ -ivk_{\parallel} e^{i\phi_{\vec{k}}} \end{pmatrix} \quad (21)$$

which is then identical with that given in [32, 10].

Since the magnetic moment is a crucial quantity determining many physical properties of the system, let us also obtain \vec{m}_2 in terms of $\vec{\rho}$. We note that $m_{2z} \propto P_- s_z$, and similarly for the other components. For later convenience, let us define (*c.f.* (10))

$$W_{2,\vec{k}} \equiv \frac{(E_{\vec{k}} + vk_{\parallel}) - (m + iv_z k_z)}{\sqrt{2}\mathcal{N}_{\vec{k}}} \quad (22)$$

We easily find

$$|W_{2,\vec{k}}| = [\frac{1}{2}(1 - \frac{m}{E_{\vec{k}}})]^{1/2}. \quad (23)$$

Note that $|W_{\vec{k}}|^2 + |W_{2,\vec{k}}|^2 = 1$ for any \vec{k} . As before, we can replace $E_{\vec{k}}$ by the chemical potential μ for states on the Fermi surface, and shall again drop the subscripts \vec{k} if no confusion can arise. At the Fermi level for electron doped Bi_2Se_3 , we have thus $|W_2| > 1/\sqrt{2}$.

We have, using (6), (7) and (16),

$$P_-|\vec{k}, \alpha\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \left(\frac{W^*W_2}{|W|}|\hat{k}+\rangle + ie^{i\phi_{\vec{k}}} \frac{WW_2^*}{|W|}|\hat{k}-\rangle \right) \quad (24)$$

and

$$P_-|\vec{k}, \beta\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \left(-ie^{-i\phi_{\vec{k}}} \frac{W^*W_2}{|W|}|\hat{k}+\rangle - \frac{WW_2^*}{|W|}|\hat{k}-\rangle \right) \quad (25)$$

where $|\hat{k}\pm\rangle$ are the spin wavefunctions defined in (12) and (13). Defining the phase $\chi_{\vec{k}}$ by

$$e^{i\chi_{\vec{k}}} = \frac{WW_2^*}{|W||W_2|} \quad (26)$$

We have $\chi_{\vec{k}} = \tan^{-1} \frac{v_z k_z}{v k_{\parallel}}$, and is thus basically the polar angle of \vec{k} if we rescale the anisotropic Fermi surface to a sphere. From (24) and (25) and noting $P_{-s_{x,y,z}} = P_{-s_{x,y,z}}P_-$, we easily find

$$m_{2z}(\vec{k}) = g_{2z}|W_2|^2 \left[-\cos(2\chi_{\vec{k}})\rho_z + \sin(2\chi_{\vec{k}}) \begin{pmatrix} 0 & e^{-i\phi_{\vec{k}}} \\ e^{i\phi_{\vec{k}}} & 0 \end{pmatrix} \right] \quad (27)$$

$$\begin{aligned} m_{2x}(\vec{k}) = g_{2p}|W_2|^2 & \left[-\sin(2\chi_{\vec{k}})\cos(\phi_{\vec{k}})\rho_z - \sin\phi_{\vec{k}} \begin{pmatrix} 0 & -ie^{-i\phi_{\vec{k}}} \\ ie^{i\phi_{\vec{k}}} & 0 \end{pmatrix} \right. \\ & \left. - \cos(2\chi_{\vec{k}})\cos\phi_{\vec{k}} \begin{pmatrix} 0 & e^{-i\phi_{\vec{k}}} \\ e^{i\phi_{\vec{k}}} & 0 \end{pmatrix} \right] \end{aligned} \quad (28)$$

$$\begin{aligned} m_{2y}(\vec{k}) = g_{2p}|W_2|^2 & \left[-\sin(2\chi_{\vec{k}})\sin(\phi_{\vec{k}})\rho_z + \cos\phi_{\vec{k}} \begin{pmatrix} 0 & -ie^{-i\phi_{\vec{k}}} \\ ie^{i\phi_{\vec{k}}} & 0 \end{pmatrix} \right. \\ & \left. - \cos(2\chi_{\vec{k}})\sin\phi_{\vec{k}} \begin{pmatrix} 0 & e^{-i\phi_{\vec{k}}} \\ e^{i\phi_{\vec{k}}} & 0 \end{pmatrix} \right] \end{aligned} \quad (29)$$

The above results are more transparent if we introduce

$$\rho_r = \cos\phi_{\vec{k}}\rho_x + \sin\phi_{\vec{k}}\rho_y \quad (30)$$

$$\rho_{\phi} = -\sin\phi_{\vec{k}}\rho_x + \cos\phi_{\vec{k}}\rho_y \quad (31)$$

as the “radial” and “azimuthal” components of $\vec{\rho}$ and similarly for \vec{m}_2 . We have

$$m_{2z}(\vec{k}) = g_{2z}|W_2|^2 \left[-\cos(2\chi_{\vec{k}})\rho_z + \sin(2\chi_{\vec{k}})\rho_r \right] \quad (32)$$

$$m_{2r}(\vec{k}) = g_{2p}|W_2|^2 \left[-\sin(2\chi_{\vec{k}})\rho_z - \cos(2\chi_{\vec{k}})\rho_r \right] \quad (33)$$

and

$$m_{2\phi}(\vec{k}) = g_{2p}|W_2|^2 [\rho_{\phi}] \quad (34)$$

with the symmetries manifest (note that $\chi_{\vec{k}}$ is odd under $k_z \rightarrow -k_z$).

The form of \vec{m}_2 is somewhat more complicated than \vec{m}_1 , which unfortunately is the price we have to pay since we used \vec{m}_1 to construct our basis. We note that, according to [34], g_{2z} and g_{2p} can in some instances be large compared with g_{1z} and g_{1p} , for example for Sb_2Te_3 .

2.2. another alternative basis

As mentioned, we can choose any quantity that transform as a pseudovector to aid our construction of the pseudospins. As an example, we here try using instead $\frac{1-\sigma_x}{2}\vec{s} = P_- \vec{s}$. Following the same procedure as subsection 2.1, we first evaluate

$$P_- |\vec{k}, \alpha'\rangle = \frac{W_2}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \begin{pmatrix} 1 \\ ie^{i\phi_{\vec{k}}} \end{pmatrix} \quad (35)$$

and

$$P_- |\vec{k}, \beta'\rangle = -\frac{W_2^*}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \begin{pmatrix} ie^{-i\phi_{\vec{k}}} \\ 1 \end{pmatrix} \quad (36)$$

The matrix for $P_- s_z$ then becomes, in $|\vec{k}, \alpha'\rangle$ and $|\vec{k}, \beta'\rangle$ space

$$\begin{pmatrix} 0 & -ie^{-i\phi_{\vec{k}}} W_2^{*2} \\ ie^{i\phi_{\vec{k}}} W_2^2 & 0 \end{pmatrix}$$

With the same logic as before, we see that the proper choice for $|\vec{k}, \alpha\rangle_2$ (we distinguish our new basis in this section by the subscript 2) should be

$$|\vec{k}, \alpha\rangle_2 = \frac{i}{\sqrt{2}} \left(\frac{W_2^*}{|W_2|} |\vec{k}, \alpha'\rangle + ie^{i\phi_{\vec{k}}} \frac{W_2}{|W_2|} |\vec{k}, \beta'\rangle \right) \quad (37)$$

and from $|\vec{k}, \beta\rangle_2 \equiv TP|\vec{k}, \alpha\rangle_2$, we have

$$|\vec{k}, \beta\rangle_2 = -\frac{i}{\sqrt{2}} \left(ie^{-i\phi_{\vec{k}}} \frac{W_2^*}{|W_2|} |\vec{k}, \alpha'\rangle + \frac{W_2}{|W_2|} |\vec{k}, \beta'\rangle \right) \quad (38)$$

Note the sign changes as well as the extra factors of $\pm i$ compared with (16) and (17). Explicitly, we have

$$P_- |\vec{k}, \alpha\rangle_2 = i \frac{|W_2|}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (39)$$

$$P_- |\vec{k}, \beta\rangle_2 = i \frac{|W_2|}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (40)$$

which results in simple expressions for \vec{m}_2 :

$$m_{2z}(\vec{k}) = g_{2z} |W_2|^2 \rho_{2z} \quad (41)$$

$$m_{2x}(\vec{k}) = g_{2p} |W_2|^2 \rho_{2x} \quad (42)$$

$$m_{2y}(\vec{k}) = g_{2p} |W_2|^2 \rho_{2y} \quad (43)$$

where we have denoted Pauli matrices in $|\vec{k}, \alpha\rangle_2 |\vec{k}, \beta\rangle_2$ space by $\rho_{2,x,y,z}$. This basis has thus the advantage of having simpler forms for the magnetic moments if g_{2z} and g_{2p} dominate over g_{1z} and g_{1p} , or if $|W_2|$ is large compared with $|W|$. However there is a disadvantage. Explicit calculation shows that, for \vec{k} residing in the northern hemisphere,

$$|\vec{k}, \alpha\rangle_2 = \frac{i}{2E_{\vec{k}}[1 - \frac{m}{E_{\vec{k}}}]^{1/2}} \begin{pmatrix} E_{\vec{k}} - m + iv_z k_z \\ ivk_{\parallel} e^{i\phi_{\vec{k}}} \\ -(E_{\vec{k}} + m - iv_z k_z) \\ ivk_{\parallel} e^{i\phi_{\vec{k}}} \end{pmatrix} \quad (44)$$

Since $|\vec{k}, \alpha\rangle_2$ in the southern hemisphere is dictated by $|\vec{k}, \alpha\rangle_2 = P|\vec{k}, \alpha\rangle_2$, one can check that this pseudospin basis for the single particle has a discontinuity (sign change) across the equator, hence extra caution is necessary when calculations are made which involves, e.g., scattering between these states. Note however the Cooper pair wavefunction, when expressed in terms of this basis, would *not* suffer from any artificial discontinuity across the equator, since the Cooper pairs involve both \vec{k} and $-\vec{k}$.

3. Conclusion

In conclusion, we have presented a slight generalization of the method in Ref [22] for constructing the pseudospin basis of a time-reversal and inversion symmetric system. We have also shown how it can generate the “manifestly covariant Bloch basis” of Ref [31, 32, 10] in the example given by (1). We emphasize once more that the method of [22] is applicable beyond (1), in particular it is not restricted to the number of orbitals involved.

4. Acknowledgements

This research is supported by the Ministry of Science and Education of Taiwan under grant numbers MOST-103-2119-M001-011-MY2 and MOST-104-2112-M-001-006-MY3.

References

- [1] Hor Y S, Williams A J, Checkelsky J G, Roushan P, Seo J, Xu Q, Zandergern H W, Yazdani A, Ong N P, and Cava R J, *Phys. Rev. Lett.* 104, 057001 (2010)
- [2] Wray L A, Xu S-Y, Xia Y, Hor Y S, Qian D, Fedorov A V, Lin H, Bansil A, Cava R J, and Hasan M Z, *Nat. Phys.* 6, 855 (2010).
- [3] Kriener M, Segawa K, Ren Z, Sasaki S, and Ando A, *Phys. Rev. Lett.* 106, 127004 (2011)
- [4] Liu Z H, Yao X, Shao J, Zuo M, Pi L, Tan S, Zhang C, and Zhang Y H, *J. Am. Chem. Soc.* 137, 10512 (2015).
- [5] Fu L and Berg E, *Phys. Rev. Lett.* 105, 097001 (2010)
- [6] Sasaki S, Kriener M, Segawa K, Yada K, Tanaka Y, Sato M, and Ando Y, *Phys. Rev. Lett.* 107, 217001 (2011).
- [7] Levy N, Zhang T, Ha J, Sharifi F, Talin A A, Kuk Y and Strosio J A, *Phys. Rev. Lett.* 110, 117001 (2013)
- [8] Peng H, De D, Lv B, Wei F and Chu C-W, *Phys. Rev. B* 88, 024515 (2013)
- [9] Fu L, *Phys. Rev. B*, 90, 100509(R), (2014)
- [10] Venderbos J W F, Kozii V and Fu L, arXiv:1512.04554
- [11] Matano K, Kriener M, Segawa K, Ando Y and Zheng G-q, *Nat. Phys.* (2016)
- [12] Pan Y, Nikitin A M, Araizi G K, Huang Y K, Matsushita Y, Naka T and deVisser A, *Sci. Rep.* 6, 28632 (2016)
- [13] Yonezawa S, Tajiri K, Nakata S, Nagai Y, Wang Z, Segawa K, Ando A and Maeno Y, arXiv:1602.08941
- [14] Kriener M, Segawa K, Sasaki S and Ando Y, *Phys. Rev. B* 86, 180505(R), (2012)
- [15] Sandilands L J, Reijnders A A, Kriener M, Segawa K, Sasaki S, Ando Y and Burch K S, *Phys. Rev. B* 90, 094503 (2014)
- [16] Brydon P M R, Das Sarma S, Hui H-Y, Sau J D, *Phys. Rev. B* 90, 184512 (2014)

- [17] Wan X and Savrasov S Y, *Nat. Commun.* 5, 4144 (2014)
- [18] Hao L and Lee T K, *Phys. Rev. B* 83, 134516 (2011)
- [19] Hsieh T H and Fu L, *Phys. Rev. Lett.* 108, 107005 (2012).
- [20] Yamakage A, Yada K, Sato M and Tanaka Y, *Phys. Rev. B* 85, 180509(R) (2012)
- [21] Lahoud E, Maniv E, Shaviv Petrushevsky M, Naamneh M, Ribak A, Wiedmann W, Petaccia L, Salman Z, Chashka K B, Dagan Y and Kanigel A, *Phys. Rev. B* 88, 195107 (2013)
- [22] Yip S-K, *Phys. Rev. B* 87, 104505 (2013)
- [23] Anderson P W, *Phys. Rev. B* 30, 1549 (1984)
- [24] Volovik G E and Gorkov L P, *Pis'ma Zh. Eksp. Teor. Fiz.* 39, 550 (1984) [*JETP Lett.* 39, 674 (1984)]; *Zh. Eksp. Teor. Fiz.* 88, 1412 (1985) [*Sov. Phys JETP* 61, 843 (1985)].
- [25] Ueda K and Rice T M, *Phys. Rev. B* 31, 7114 (1985).
- [26] Blount E I, *Phys. Rev. B* 32, 2935 (1985).
- [27] Sigrist M and Ueda K, *Rev. Mod. Phys.* 63, 239 (1991)
- [28] Yip S and Garg A, *Phys. Rev. B* 48, 3304 (1993)
- [29] Joynt R and Taillefer L, *Rev. Mod. Phys.* 74, 235 (2002)
- [30] Yip S-K, *Annu. Rev. Cond. Matter Physics.* 5:15-33 (2014)
- [31] Fu L, *Phys. Rev. Lett.* 115, 026401 (2015)
- [32] Kozii V and Liang L, *Phys. Rev. Lett.* 115, 207002 (2015)
- [33] Takami S, Yada K, Yamakage Ai, Sato M, and Tanaka Y *J. Phys. Soc. Japan* 83 064705 (2014); Nagai Y, Nakamura H, and Machida M *J. Phys. Soc. Japan* 83 053705 (2014); Hao L and Lee T K, *J. Phys.: Condens. Matter* 27, 105701 (2015)
- [34] Liu C-X, Qi X L, Zhang H J, Dai X, Fang Z and Zhang S C, *Phys. Rev. B* 82, 045122 (2010)